=>

Uploading C:\Program Files\Stnexp\Queries\10692735.str

chain nodes :

10 11 12 13 17 18 19

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

7-10 7-18 8-11 8-19 11-12 11-17 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

5-7 6-9 7-8 7-10 7-18 8-9 8-11 8-19 11-17 12-13

exact bonds :

11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:Cy,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 17:CLASS 18:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

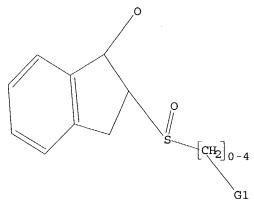
=> que L1

L2 QUE L1

=> d

L2 HAS NO ANSWERS

L1 STR



G1 Cy,Ak

Structure attributes must be viewed using STN Express query preparation. L2 QUE ABB=ON PLU=ON L1

=> s 12

SAMPLE SEARCH INITIATED 14:37:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 721 TO ITERATE

100.0% PROCESSED 721 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 12810 TO 16030

PROJECTED ANSWERS: 4 TO 200

- Into Horizon

L3 4 SEA SSS SAM L1

=> d scan

L3 4 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1H-Inden-1-ol, 5-azido-2,3-dihydro-2-(methylsulfonyl)-, acetate (ester)

(9CI)

MF C12 H13 N3 O4 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s 12 full -

FULL SEARCH INITIATED 14:37:56 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 14788 TO ITERATE

69 ANSWERS

```
100.0% PROCESSED 14788 ITERATIONS SEARCH TIME: 00.00.01
```

L4 69 SEA SSS FUL L1

=>

=>

=> s 14 and sulfox?

9366 SULFOX?

L5 0 L4 AND SULFOX?

=> s l4 and sulfo?

1667899 SULFO?

L6 39 L4 AND SULFO?

=> s 14 not 16

L7 30 L4 NOT L6

=> d scan

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-,

 $[1\alpha, 2\beta(R^*)]$ - (9CI)

MF C15 H13 Cl O2 S

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-,

 $[1\alpha, 2\alpha(S^*)]$ - (9CI)

MF C15 H13 Cl O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN IN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-,

 $[1\alpha, 2\beta(S^*)]$ - (9CI) MF C16 H16 O2 S

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

MF C16 H16 O2 S

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-, $[1\alpha, 2\alpha(S^*)]$ - (9CI)

MF C16 H16 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7

30 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI) C15 H13 Cl O2 S

L8 22 L7

=> d ibib abs hitstr 1-22

L8 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:202618 CAPLUS

DOCUMENT NUMBER: 138:221365

TITLE: Preparation of indan-1-ols as appetite depressants

INVENTOR(S): Jaehne, Gerhard; Krone, Volker; Bickel, Martin;

Gossel, Matthias

PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany

SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

GΙ

```
PATENT NO.
                          KIND
                                DATE
                                                  APPLICATION NO.
                                                  ______
      WO 2003020696
                                20030313
                                                  WO 2002-EP9206
                          Α1
                                                                      20020817
          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
               CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
               GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
               LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
               \mathtt{PL},\ \mathtt{PT},\ \mathtt{RO},\ \mathtt{RU},\ \mathtt{SD},\ \mathtt{SE},\ \mathtt{SG},\ \mathtt{SI},\ \mathtt{SK},\ \mathtt{SL},\ \mathtt{TJ},\ \mathtt{TM},\ \mathtt{TN},\ \mathtt{TR},\ \mathtt{TT},\ \mathtt{TZ},
               UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
               CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
               PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR,
               NE, SN, TD, TG
      DE 10142667
                          A1
                                20030327
                                                  DE 2001-10142667 20010831
      US 2003114681
                           Α1
                                20030619
                                                  US 2002-231394
                                                                      20020830
      US 6657086
                          B2
                                20031202
      US 2004068016
                           A1
                                20040408
                                                  US 2003-665021
                                                                      20030922
PRIORITY APPLN. INFO.:
                                                                      20010831
                                               DE 2001-10142667 A
                                               US 2002-231394
                                                                 A3 20020830
OTHER SOURCE(S):
                             MARPAT 138:221365
```

$$\mathbb{R}^3$$
 OH OH \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb

AB Title compds. I [R1, R2, R3, R4 = H, halo, CN, etc.; X = S, SO, SO2; Y = (CH2)p; p = 0-3; R5 = CF3, alkyl, cycloalkyl] and their pharmaceutically acceptable salts were prepared For example, NaBH4 mediated reduction of 5-chloro-2-methylsulfonylindan-1-one, e.g., prepared from 2-bromo-5-chloroindan-1-one in 2-steps, provided indanol II. In milk consumption studies with female NMRI mice, indanol II exhibited very good

anorectic effects, i.e., 50% decrease in milk consumption verses control. IT 500910-96-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of indanols as appetite depressants) 500910-96-3 CAPLUS

CN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylsulfinyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:202465 CAPLUS

DOCUMENT NUMBER:

138:221361

TITLE:

RN

Preparation of indan-1-ols for producing drugs for the

prophylaxis or treatment of obesity

INVENTOR(S):

Jaehne, Gerhard; Krone, Volker; Bickel, Martin;

Gossel, Matthias

PATENT ASSIGNEE(S):

Aventis Pharma Deutschland G.m.b.H., Germany

SOURCE:

PCT Int. Appl., 52 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

· 1

PATENT INFORMATION:

| WO 2003020263 Al 20030313 WO 2002-EP9205 20020817 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 Al 20030320 DE 2001-10142666 20010831 US 2003134879 Al 20030717 US 2002-231183 20020830 | | | | | | | | | |
|--|----------|--|--|--|--|--|--|--|--|
| CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 Al 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 Al 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 Al 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 A1 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 A1 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 A1 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 A1 20030320 DE 2001-10142666 20010831 | [| | | | | | | | |
| PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 10142666 A1 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| NE, SN, TD, TG DE 10142666 A1 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| DE 10142666 A1 20030320 DE 2001-10142666 20010831 | | | | | | | | | |
| | | | | | | | | | |
| US 2003134879 A1 20030717 US 2002-231183 20020830 | 20010831 | | | | | | | | |
| | | | | | | | | | |
| PRIORITY APPLN. INFO.: DE 2001-10142666 A 20010831 | | | | | | | | | |
| OTHER SOURCE(S): MARPAT 138:221361 | | | | | | | | | |
| GI | | | | | | | | | |

AB Title compds. [I; R1-R4 = H, F, Cl, Br, I, cyano, N3, N02, OH, alkoxy, cycloalkoxy, benzyloxy, phenoxy, alkylcarbonyloxy, etc.; X = S, S0, S02; Y = (CH2)p; p = 0-3; R5 = CF3, (fluorinated) alkyl, cycloalkyl, etc.], were prepd for producing a drug for body weight loss of mammals. Thus, 5-chloro-2-methylsulfonylindan-1-one (preparation given) and NaBH4 in EtOH were put into a ultrasound bath for 4 h followed by stirring with 2N HCl to give 5-chloro-2-methylsulfonylindan-1-ol. The latter at 20 mg/kg i.p. was applied in female NMRI mice and gave 50% reduction of milk consumption of the treated mice.

IT 95720-00-6P 134779-81-0P 134779-82-1P 500910-96-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indanols for producing drugs for prophylaxis or treatment of obesity)

RN 95720-00-6 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 134779-81-0 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 134779-82-1 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 500910-96-3 CAPLUS

CN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylsulfinyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:202409 CAPLUS

DOCUMENT NUMBER:

138:226750

TITLE:

Use of C2-substituted indan-1-ol derivatives in

antiobesity drugs

INVENTOR(S):

Jaehne, Gerhard; Krone, Volker; Bickel, Martin;

Gossel, Matthias

PATENT ASSIGNEE(S):

Aventis Pharma Deutschland G.m.b.H., Germany

SOURCE:

PCT Int. Appl., 54 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

German

1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | | | | KIND DATE | | | | APPLICATION NO. DATE | | | | | | | | | ÷ | |
|--|---------|------|-----|-----------|-------------|-------|-------|----------------------|-------------------------|------|------|------|-----|------|------|-----|-----|----|
| WO 2003020199 7 | | | | | A1 20030313 | | | | WO 2002-EP9199 20020817 | | | | | | | | | |
| | | | | | | | | | | | | | | BZ, | | СH | CM | |
| | ** * | | • | • | • | • | • | • | • | | • | • | • | GB, | • | • | | |
| | | • | • | • | • | - | • | | • | | • | • | | KZ, | , | • | , | |
| | | • | • | • | • | • | | • | • | • | • | | • | • | • | | • | |
| | | | • | , | | • | | • | • | • | , | • | • | NO, | • | • | , | |
| | | PL, | PT, | RO, | RU, | SD, | SE, | SG, | SI, | SK, | SL, | ΤJ, | TM, | TN, | TR, | TT, | ΤZ, | |
| | | UA, | UG, | UΖ, | VN, | ΥU, | ZA, | ZM, | ZW, | ΑM, | ΑZ, | BY, | KG, | KΖ, | MD, | RU, | ТJ, | TM |
| | RW: | GH, | GM, | KΕ, | LS, | MW, | ΜZ, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | ΑT, | BE, | BG, | |
| | | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FΙ, | FR, | GB, | GR, | IE, | IT, | LU, | MC, | NL, | |
| | | | | | | | | | | | | | | GO, | | | | |
| | | | | TD, | | , | • | • | • | • | , | • | • | ~ . | | | , | |
| DI | E 1014: | , | • | , | | 2003 | 0320 | | ומ | E 20 | 01-1 | 0142 | 660 | 2001 | 0831 | | | |
| DE 10142660 A1 20030320 DE 2001-10142660 20010831 US 2003134881 A1 20030717 US 2002-230379 20020829 | | | | | | | | | | | | | | | | | | |
| | | | | | | | | | 0. | 20 | 02 2 | 3037 | , | 2002 | 0025 | | | |
| US 6667345 B2 20031223 | | | | | | | | | | | | | | | | | | |
| PRIORITY APPLN. INFO.: DE 2001-10142660 A 20010831 | | | | | | | | | | | | | | | | | | |
| OTHER S | SOURCE | (S): | | | MAR | PAT : | 138:: | 2267 | 50 | | | | | | | | | |
| GI | | | | | | | | | | | | | | | | | | |

AB The invention relates to the use of C2-substituted indan-1-ol systems, and to the physiol. tolerable salts and the physiol. functional derivs. of the same, for producing medicaments used to reduce the weight of mammals, and for the prophylaxis or the treatment of obesity. The invention also relates to the use of compds. of formula (I), wherein the radicals have the cited designations, and to the physiol. tolerable salts and the physiol. functional derivs. of the same, for producing a medicament for the prophylaxis or the treatment of obesity. The antiobesity drugs can be combined with other active ingredients, e.g. cathine, phenylpropanolamine, amfepramone, mefenorex. Capsules, tablets, emulsions, dragees and suppositories are prepared containing the indan-1-ol derivative antiobesity drugs.

IT 500770-90-1 500770-91-2 500770-94-5

Ι

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (use of C2-substituted indan-1-ol derivs. in antiobesity drugs)

RN 500770-90-1 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, acetate, (1R,2R)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 500770-91-2 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, acetate, (1R,2S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 500770-94-5 CAPLUS

CN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylsulfinyl)-, acetate (9CI) (CA INDEX NAME)

REFERENCE COUNT:

4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:733853 CAPLUS

DOCUMENT NUMBER:

131:322537

TITLE:

Preparation of 10,11-dihydro-11-

hydroxybenz[b]indeno[2,1-e]pyran-10-ones and analogs

for enhancing biosynthesis of erythropoietin

INVENTOR(S):

Williams, Jonathan Gareth; Houck, David R.; Smith, David Edward; Rathbone, Daniel Lee; Billington, David Charles; Golding, Bernard T.; Collington, Eric W.;

Kitchin, John; Rich, Nicholas

PATENT ASSIGNEE(S):

OSI Pharmaceuticals, Inc., USA

SOURCE:

U.S., 13 pp., Cont.-in-part of U.S. 5,882,436.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. DATE |
|----------------------|------|----------|---------------------------|
| | | | |
| US 5985913 | A | 19991116 | US 1998-69693 1998042 |
| PRIORITY APPLN. INFO | . : | | US 1996-32268P P 1996112 |
| | | | US 1997-978346 A2 1997112 |

OTHER SOURCE(S):

MARPAT 131:322537

GΙ

$$R^{1}$$
 O
 R^{2}
 R^{3}
 I

AB Title compds. [I; R1,R4 = H or 1-4 of halo, alkyl, alkoxy, etc.; R2 = OR10 and R3 = H or R2R3 = O; R10 = H or alkanoyl; dashed line = optional addnl. bond] were prepared Thus, 3',5'-dimethyl-2'-hydroxy-2-methylsulfinylacetophenone (preparation given) was cyclocadensed with 2-(OHC)C6H4CHO to give I (R1 = 6,8-Me2, R2 = OH, R3 = R4 = H, dashed line = bond). Data for biol. activity of I were given.

IT 249514-81-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 10,11-dihydro-11-hydroxybenz[b]indeno[2,1-e]pyran-10-ones

and analogs for enhancing biosynthesis of erythropoietin)

RN249514-81-6 CAPLUS

Benz[b]indeno[2,1-e]pyran-10(4bH)-one, 10a,11-dihydro-11-hydroxy-6,8-CNdimethyl-10a-(methylsulfinyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2004 ACS on STN ANSWER 5 OF 22

3

ACCESSION NUMBER:

1994:409577 CAPLUS

DOCUMENT NUMBER:

121:9577

TITLE:

Reactions of $\eta 2$ -(2-acylaryl-

C,O)tetracarbonylmanganese(I) complexes with some

vinyl sulfur compounds

AUTHOR(S):

Cambie, Richard C.; Rutledge, Peter S.; Welch, David

R.; Woodgate, Paul D.

CORPORATE SOURCE:

Department of Chemistry, University of Auckland,

Private Bag 92019, Auckland, N. Z.

SOURCE:

Journal of Organometallic Chemistry (1994), 467(2),

237-44

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE:

Journal English

LANGUAGE: OTHER SOURCE(S):

CASREACT 121:9577

The thermally promoted reactions of some Ph and diterpenoid η2-(2-acylary1-C,0)tetracarbonylmanganese(I) complexes with Ph vinyl sulfone, Me vinyl sulfone, or Ph vinyl sulfoxide, have been investigated. The major products from the diterpenoid complexes arises from insertion followed by reductive demetalation; cyclopenta-annulation, when it occurs, is a minor process. Liberation of the metal-free adducts from their Mn-containing precursors requires treatment with either acid or photolysis-oxidation

IT 155519-28-1P 155519-29-2P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 155519-28-1 CAPLUS

1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-, CN (CA INDEX NAME) $(1\alpha, 2\beta)$ - (9CI)

RN 155519-29-2 CAPLUS CN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-, $(1\alpha,2\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:558285 CAPLUS

DOCUMENT NUMBER:

115:158285

TITLE:

Cooxidation reaction of indene and aromatic thiols in

the presence of ovalbumin

AUTHOR (S):

Freer, Juanita; Fuentealba, Cecilia; Gonzalez,

Elizabeth; Baeza, Jaime

CORPORATE SOURCE:

SOURCE:

Dep. Quim., Univ. Concepcion, Concepcion, Chile Phosphorus, Sulfur and Silicon and the Related

Phosphorus, Sulfur and Silicon and the Elements (1991), 61(1-2), 41-8

CODEN: PSSLEC; ISSN: 1042-6507

DOCUMENT TYPE:

LANGUAGE:

Journal English

OTHER SOURCE(S):

CASREACT 115:158285

AB The thiol olefin cooxidn. reaction (TOCO) between indene and aromatic thiols in presence of ovalbumin has been studied in hexane. While this reaction under normal conditions leads to the formation of 6 products, in the presence of OVA give stereospecifically only the trans-2-phenylmercapto-1-indanol derivative on the protein surface.

IT 32819-87-7P 32819-88-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 32819-87-7 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1R-

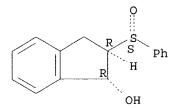
 $[1\alpha, 2\beta(R^*)]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 32819-88-8 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)-, [1R- $[1\alpha, 2\beta(S^*)]$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 7 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:539316 CAPLUS

DOCUMENT NUMBER:

115:139316

TITLE:

Fuel instability model studies: the liquid-phase

cooxidation of thiols and indene by oxygen

AUTHOR (S):

Morris, Robert E.; Mushrush, George W.

CORPORATE SOURCE:

Nav. Technol. Cent. Saf. Survivabil., Nav. Res. Lab.,

Washington, DC, 20375, USA

SOURCE:

Energy & Fuels (1991), 5(5), 744-8

CODEN: ENFUEM; ISSN: 0887-0624

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Instability problems in middle distillate fuels were correlated with the presence of both active olefin species and heteroat. compds. such as thiols. The type of S compound rather than the total S concentration is the key to

fuel instability reactions. Low concns. of thiols will act as radical traps to inhibit autoxidn. When added to a fuel, thiols accelerated the rate of Oxidation without a commensurate increase in peroxidn. Evidence for the oxidative addition of thiols to olefins was observed by studying the addition

of thiophenol to indene in a model fuel during stressing in both a model system at 100-120° and in the jet fuel thermal oxidation test apparatus at 350°. Similarities and differences were found in the 2 systems, with the product distribution being temperature dependent. This could account, in part, for the differences in thiol influences on autoxidn. observed in model systems and in fuels.

TТ 92621-28-8P

> RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in reaction of indene with thiophenol and oxygen, jet fuel instability model study in relation to)

92621-28-8 CAPLUS RN

CN1H-Inden-1-ol, 2,3-dihydro-2-(phenylsulfinyl)- (9CI) (CA INDEX NAME)

ANSWER 8 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:448966 CAPLUS

DOCUMENT NUMBER:

115:48966

TITLE:

Cooxidation between thiophenol and cyclopentene

AUTHOR (S):

Freer, Juanita; Palma, Graciela; Fuentealba, Cecilia;

Pena, Monica; Baeza, Jaime

CORPORATE SOURCE:

Dep. Quim., Univ. Concepcion, Concepcion, Chile

SOURCE:

Boletin de la Sociedad Chilena de Quimica (1991),

36(1), 11-16

CODEN: BOCQAX; ISSN: 0366-1644

DOCUMENT TYPE:

LANGUAGE:

Journal Spanish

GΙ

AB Treatment of thiophenol with cyclopentene in the presence of O2 gene adduct I (R = H) as well as cooxidn. products, i.e., cis- and trans-I (R = OH) and the sulfoxide derivs. The reaction of thiophenol with indene gave similar results.

IT 95720-00-6P 134779-81-0P 134779-82-1P

RN 95720-00-6 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

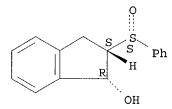
RN 134779-81-0 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 134779-82-1 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1S,2R)-rel- (9CI) (CA INDEX NAME)



L8 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1988:224013 CAPLUS

DOCUMENT NUMBER:

108:224013

TITLE:

Liquid-phase oxidation of thiophenol and indene by

tert-butyl hydroperoxide and oxygen

AUTHOR(S):

Mushruch, George W.; Watkins, John M.; Hazlett, Robert

N.; Hardy, Dennis R.; Eaton, Harold G.

CORPORATE SOURCE:

Nav. Res. Lab. Code 6180, Washington, DC, 20375-5000,

USA

SOURCE:

Fuel Science & Technology International (1988), 6(2),

165-83

CODEN: FSCTEG; ISSN: 0884-3759

DOCUMENT TYPE: LANGUAGE: Journal English

AB tert-Bu hydroperoxide (I) or O initiated the oxidation of thiophenol in the presence of indene was examined in C6H6 at 120°. The reaction is kinetically complex, but it was possible to relate the product distribution to a few competing reactions. The product mixture was determined for several reaction time periods. The product slate was similar for all time periods, but yields of the individual components varied significantly with increasing reaction time. Gaseous products included isobutylene and a trace of CH4. The major product from I was tert-BuOH. The major product observed from thiophenol was Ph2S2. Addition products included the major product 2-phenylthiyl indan. Oxidation products included indanols, indanones, and the sulfoxide and sulfone of the major product 2-phenylthiyl indan. Solvent participation was noted by trace amts. of toluene.

IT 95720-00-6P

RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in indene reaction with thiophenol and oxygen or tert-Bu hydroperoxide, jet fuel in relation to)

RN 95720-00-6 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1985:148840 CAPLUS

DOCUMENT NUMBER:

102:148840

TITLE:

Stereoselective oxidative addition of benzenethiol to

indene in the presence of ovalbumin

AUTHOR(S): CORPORATE SOURCE: Baeza, Jaime; Freer, Juanita; Palma, Graciela Dep. Quim., Univ. Concepcion, Concepcion, Chile Monatshefte fuer Chemie (1984), 115(11), 1369-71

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE:

SOURCE:

Journal English

LANGUAGE:
OTHER SOURCE(S):

CASREACT 102:148840

AB The oxidative addition of PhSH to indene in the presence of ovalbumin produces only trans-anti-2-phenylsulfinyl-1-indanol. This reaction may be considered as a biomimetic model of detoxification of certain hydrocarbons by the liver.

IT 95720-00-6

RL: PROC (Process)

(stereospecific formation of, in presence of ovalbumin)

RN 95720-00-6 CAPLUS

CN 1H-Inden-1-ol, 2,3-dihydro-2-[(R)-phenylsulfinyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1978:190435 CAPLUS

DOCUMENT NUMBER:

88:190435

TITLE:

Thiol-olefin cooxidation reaction. 6. A new

convenient route to 1-substituted indenes. Indenone

as dienophile in Diels-Alder reactions Szmant, H. Harry; Nanjundiah, Raghunath

CORPORATE SOURCE:

Dep. Chem. Chem. Eng., Univ. Detroit, Detroit, MI, USA

SOURCE:

AUTHOR(S):

Journal of Organic Chemistry (1978), 43(9), 1835-7

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 88:190435

AB 2-(4-Chlorophenylsulfinyl)-1-indanone was decomposed in refluxing toluene to give indenone which was trapped by cyclopentadiene, hexachlorocyclopentadiene, and anthracene to give the resp. Diels-Alder adducts.

IT 62967-56-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, 1-indanone analog from)

RN 62967-56-0 CAPLUS

CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

65495-98-9P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN65495-98-9 CAPLUS

CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, acetate (9CI) (CA INDEX NAME)

ANSWER 12 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1977:422824 CAPLUS

DOCUMENT NUMBER:

87:22824

TITLE:

SOURCE:

A new route to 1,2-indanedione

AUTHOR(S):

Szmant, H. Harry; Nanjundiah, Raghunath

CORPORATE SOURCE:

Dep. Chem. Chem. Eng., Univ. Detroit, Detroit, MI, USA

Organic Preparations and Procedures International

(1977), 9(1), 35-8

CODEN: OPPIAK; ISSN: 0030-4948

DOCUMENT TYPE:

Journal LANGUAGE: English

OTHER SOURCE(S):

CASREACT 87:22824

AΒ O was bubbled through a mixture of indene and p-ClC6H4SH in isooctane at room temperature and the resultant mixture of isomeric indanol sulfoxides (I;

X = CHOH; R = H; R1 = p-ClC6H4SO) was oxidized with Jones reagent to give indanone sulfoxide (I; X = CO; R and R1 as before), which was refluxed with MeOH in the presence of iodine and the product (I; X = CO; R = R1 =OMe) was deketalized with EtOH-H2SO4 at reflux to give 1,2-indandione [I; X = CO; (RR1) = O].

IT 62967-56-0P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and Jones oxidation of)

RN62967-56-0 CAPLUS

1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro- (9CI) CN NAME)

L8 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1977:170438 CAPLUS

DOCUMENT NUMBER:

86:170438

TITLE:

The thiol-olefin cooxidation (TOCO) reaction. IV. Temperature effects on product distribution in the

TOCO reaction of indene and aromatic thiols

AUTHOR (S):

Szmant, H. H.; Mata, A. J.; Namis, A. J.;

Panthananickal, A. M.

CORPORATE SOURCE:

Dep. Chem., Univ. Detroit, Detroit, MI, USA

SOURCE:

Tetrahedron (1976), 32(22), 2665-80

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The stereochem. of the TOCO reaction of indene with RC6H4SH (R=4-Cl, 4-MeO, 3-Me) is temperature dependent. Increasing amts. of cis addition products

are formed as the temperature is lowered to -23° and raised to .apprx.60°. The sensitivity of the temperature effect depends on the electronic character of the substituent in RC6H4SH. The effect of solvent, addition of cumyl hydroperoxide, K2S2O8, galvinoxyl, PhNoCMe3, Na2S2O3, and Na tetrathionate, and the kinetics of the TOCO reaction were determined

IT 62703-00-8P 62703-01-9P 62703-02-0P

62703-05-3P 62703-06-4P 62703-07-5P

62703-10-0P 62703-11-1P 62703-12-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 62703-00-8 CAPLUS

CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, $[1\alpha, 2\beta(S^*)]$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 62703-01-9 CAPLUS

CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, $[1\alpha,2\beta(R^*)]$ - (9CI) (CA INDEX NAME)

RN 62703-02-0 CAPLUS CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)sulfinyl]-2,3-dihydro-, [1α ,2 α (S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 62703-05-3 CAPLUS CN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-, [1α ,2 β (S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 62703-06-4 CAPLUS CN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-, [1 α ,2 β (R*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 62703-07-5 CAPLUS CN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)sulfinyl]-,

$$[1\alpha, 2\alpha(S^*)]$$
 - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 62703-10-0 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-,

 $[1\alpha, 2\beta(S^*)]$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 62703-11-1 CAPLUS CN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-, [1 α ,2 β (R*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 62703-12-2 CAPLUS CN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)sulfinyl]-, [1 α ,2 α (S*)]- (9CI) (CA INDEX NAME)

Uploading C:\Program Files\Stnexp\Queries\10692735.str

chain nodes :
10 11 12 13 17 18 19
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
7-10 7-18 8-11 8-19 11-12 11-17 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 7-10 7-18 8-9 8-11 8-19 11-17 12-13
exact bonds :
11-12
normalized bonds :

G1:Cy,Ak

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 17:CLASS 18:CLASS 19:CLASS

L4 STRUCTURE UPLOADED

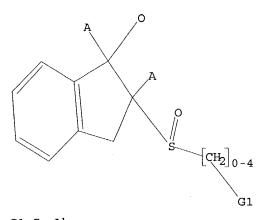
1-2 1-6 2-3 3-4 4-5 5-6

=> que L4

L5 QUE L4

=> d L5 HAS NO ANSWERS

L4 STR



G1 Cy,Ak

L6

Structure attributes must be viewed using STN Express query preparation. L5 QUE ABB=ON PLU=ON L4

=> s 15 full FULL SEARCH INITIATED 16:30:51 FILE 'BEILSTEIN' FULL SCREEN SEARCH COMPLETED - 4755 TO ITERATE

100.0% PROCESSED 4755 ITERATIONS SEARCH TIME: 00.00.07

0 ANSWERS

SEARCH IIME: 00.00.0

0 SEA SSS FUL L4